

Planar Channeling of 855 MeV Electrons in Silicon: Monte-Carlo Simulations

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Abstract. A new Monte Carlo code for the simulation of the channeling of ultrarelativistic charged projectiles in single crystals is presented. A detailed description of the underlying physical model and the computation algorithm is given. First results obtained with the code for the channeling of 855 MeV electrons in Silicon crystal are presented. The dechanneling lengths for (100), (110) and (111) crystallographic planes are estimated. In order to verify the code, the dependence of the intensity of the channeling radiation on the crystal dimension along the beam direction is calculated. A good agreement of the obtained results with recent experimental data is observed.

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1. Introduction

In this article we consider planar channeling of 855 MeV electrons in Silicon crystal using a new Monte-Carlo code.

Channeling takes place if charged particles enter a single crystal at small angle with respect to crystallographic planes or axes [1]. The particles get confined by the interplanar or axial potential and move preferably along the corresponding crystallographic planes or axes following their shape.

Recent revival of the interest to this phenomenon is due to its growing practical application. In particular, the crystals with bent crystallographic planes are used to steer high-energy charged particle beams replacing huge dipole magnets. Since its appearance [2] and first experimental verification [3] this idea has been attracting a lot of interest worldwide. Bent crystal have been routinely used for beam extraction in the Institute for High Energy Physics, Russia [4]. Series of experiment on the bent crystal deflection of proton and heavy ion beams were performed at different accelerators [5, 6, 7, 8, 9] throughout the world. The bent crystal method has been proposed to extract particles from the beam halo at CERN Large Hadron Collider [10]. The possibility to deflect positron [11] and electron [9, 12, 13] beams has been studied as well.

Another very promising application of the channeling phenomenon is a novel source of hard electromagnetic radiation. A single crystal with periodically bent crystallographic planes can force channeling particles to move along nearly sinusoidal trajectories and radiate in hard X and gamma ray frequency range. The feasibility of such a device, known as the 'crystalline undulator', was demonstrated theoretically a decade ago [14, 15] (further developments as well as historical references are reviewed in [16]). The advantage of the crystalline undulator is in extremely strong electrostatic fields inside a crystal, which are able to steer the particles much more effectively than even the most advanced superconductive magnets. This fact allows to make the period λ_u of the crystalline undulator in the hundred or even ten micron range, which is two to three orders of magnitude smaller than that of conventional undulator. Therefore the wavelength of the produced radiation $\lambda \sim \lambda_u/(2\gamma^2)$ ($\gamma \sim 10^3$ – 10^4 being the Lorentz factor of the particle) can reach the (sub)picometer range, where conventional sources with comparable intensity are unavailable [17].

Initially, it was proposed to use positron beams in the crystalline undulator. Positively charged particles are repelled by the crystal nuclei and, therefore, they move between the crystal planes, where there are no atomic nuclei and the electron density is less than average. This reduces the probability of random collisions with the crystal constituents. Hence, the transverse momentum of the particle increases slowly and the particle travels a longer distance in the channeling regime.

More recently, an electron based crystalline undulator has been proposed [18]. On one hand, electrons are less preferable than positrons. Due to their negative charge, the electrons are attracted by the lattice ions and, therefore, are forced to oscillate around the crystal plane in the process of channeling. The probability of collisions with

crystal constituents is enhanced. Thus, the dechanneling length is smaller by about two orders of magnitude in comparison to that of positrons at the same conditions. On the other hand, the electron beams are easier available and are usually of higher intensity and quality. Therefore, from the practical point of view, electron based crystalline undulator has its own advantages and deserves a thorough investigation.

There is another reason why electron channeling needs a thorough analysis. This is the disagreement between theory and experimental data. For example, the Baier-Katkov-Strakhovenko formula for the dechanneling length (equation (10.1) in [19]), L_d , predicts $L_d = 23 \mu\text{m}$ for 1.2 GeV electrons in Si (110) planar channel, while the measured value is $L_d = 28 \mu\text{m}$ [20].

For lower energies, the discrepancy is much more dramatic: $L_d = 6.7 \mu\text{m}$ calculated vs. $L_d = 31 \mu\text{m}$ measured [21] and $L_d \approx 1 \mu\text{m}$ calculated vs. $L_d = 36 \mu\text{m}$ measured [22] for electron energies 350 MeV and 54 MeV, respectively.

Clearly, further theoretical and experimental investigations of the electron channeling are necessary (see also [23]). No accurate theoretical description of the electron deflection by bent crystals or the electron-based crystalline undulator is possible until an adequate and experimentally verified theoretical or numerical model of electron channeling is available.

To build such a model, we developed a new Monte-Carlo code that allows to simulate the particle channeling and calculate the emitted radiation. In contrast to other channeling codes [24, 25, 26], our algorithm does not use the continuous potential approximation. This novel feature is especially beneficial in the case of negatively charged projectiles, which channel in the vicinity of the atomic nuclei, where the continuous potential approximation becomes less accurate.

In this paper we present the first results obtained with our code. We have studied the channeling of 855 MeV electrons in a straight single crystal of Silicon along three different crystallographic planes: (100), (110) and (111). The parameters of the simulation correspond to the conditions of the channeling experiments at Mainz Microtron (Germany) [27]. To verify our results, we calculated the dependence of the intensity of the channeling radiation on the crystal dimension along the beam direction and compared to the experimental data.

2. The Underlying Physical Model and its Validity Domain

Our model is intended for studying the interaction of ultrarelativistic projectiles with single crystals. It is best suited for light projectiles: electrons and positrons, but it can be also used for ultrarelativistic heavy projectiles.

Due to the high speed of the projectile, its interaction time with a crystal atom is very short. The atomic electrons have no time to move during the interaction. As a result, the projectile ‘sees’ a ‘snapshot’ of the atom: the atomic electrons are seen as point-like charges at fixed positions around the nucleus (see Figure 1).

The probability density to see the atomic electrons at positions $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z$ (Z

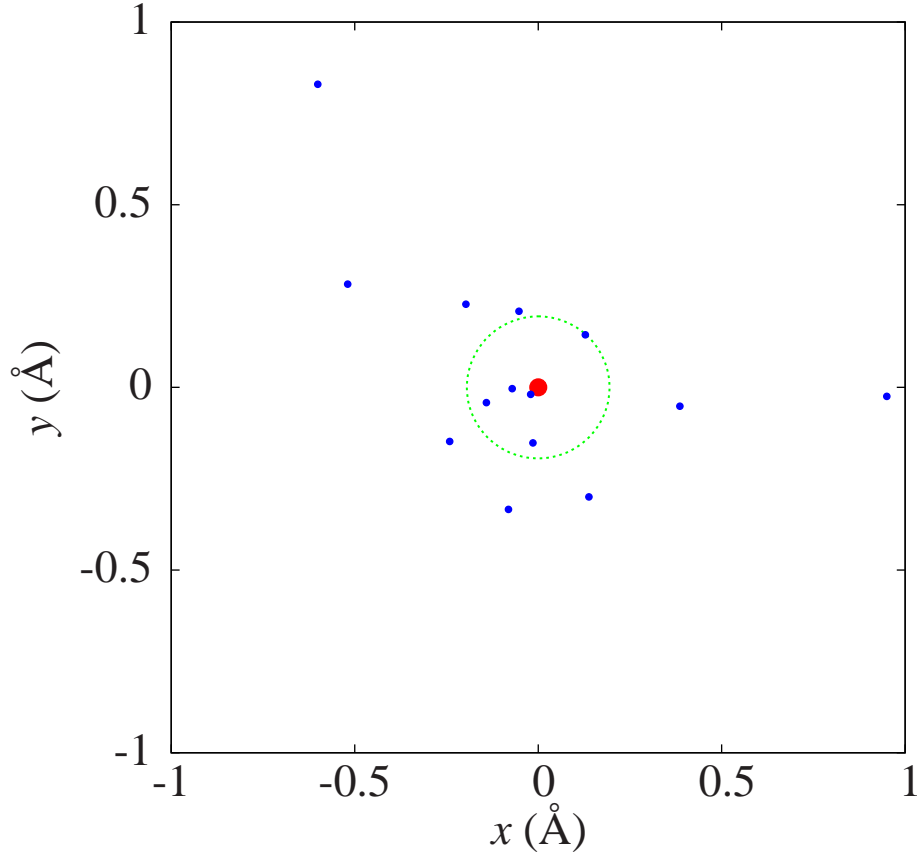


Figure 1. An example of a ‘snapshot’ of a Silicon atom as it is seen by an ultrarelativistic projectile moving along z -axis. The larger and smaller circles represent the nucleus and the electrons, respectively. The dashed line shows the Thomas-Fermi radius of the atom.

is the atomic number) is given by squared absolute value of the wave function of the atom:

$$w(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z) = |\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z)|^2. \quad (1)$$

Instead of using the exact wave function, we approximate it by a spherical symmetric probability distribution that on average reproduces the electrostatic potential of the atom in Molière’s approximation [28]. Our approach ignores nonsphericity of electron orbitals as well as anticorrelations, due to Coulomb’s repulsion and Pauli’s principle, between electron positions.

The interaction of the projectile with an atomic constituent is considered as a classical scattering in a Coulomb field of a static point-like charge. A projectile with electric charge q_p and initial speed v along z -axis attains after interaction with a static charge q_t a transverse momentum

$$\Delta \vec{p}_\perp = -q_p q_t \frac{\vec{r}_\perp}{v \vec{r}_\perp^2}, \quad (2)$$

\vec{r}_\perp is the vector connecting the projections of the projectile and the static charge onto the (xy) -plane.

The total transverse momentum attained by the projectile in the collision with the atom is a vector sum of (2) over all atom constituents. The absolute value of the projectile momentum remains unchanged. This means that the projectile energy losses for ionisation or excitation of the atom are neglected. Indeed, the ionization losses of high energy electrons or positrons in matter are very small (see, for example, Figure 27.10 in [29]).

The above procedure is approximate. It is valid if the scattering angle $\vartheta = |\Delta\vec{p}_\perp|/p$ is small. In the opposite case, not only formula (2) but also the representation of the atom as a collection of static charges become wrong. However, accurate description of the large angle scattering is not important for modelling of the channeling processes. First, such processes are rare. Second, if the projectile is scattered by an angle that is much larger than the critical (Lindhard's) angle ϑ_L [1], its probability to return to the channeling regime is negligible. Therefore the trajectory of a projectile after a large-angle scattering is out of our interest and the precise value of the large scattering angle does not matter.

On the other hand, the scattering by $\vartheta \lesssim \vartheta_L$ is important for a proper modelling of the channeling phenomenon. Lindhard's angle for ultrarelativistic projectiles is typically of submilliradian range. The described procedure as well as formula (2) are valid for such small scattering angles.

The 'snapshot' model is applied not only to each atom but also to the crystal as a whole. The thermal motion of the atoms is even slower than the motion of atomic electrons. Therefore, the projectile sees the atomic nuclei 'frozen' at random positions in the vicinity of nodes of the crystal lattice. The probability distribution of the position of the nucleus relative to the node can be approximated by a three dimensional normal distribution with the variance equal to the squared amplitude of thermal vibrations of the crystal atoms.

Although the crystal constituents are considered as static point-like charges, and the model looks like completely classical construction at the first sight, the quantum properties of the crystal are properly taken into account: the probability distributions of electrons and nuclei are found from the quantum theory.

In contrast, the quantum aspects of the projectile motion are indeed completely ignored. Our code performs calculation of trajectories of the projectiles in the crystal. Calculation of a particle trajectory implies that its coordinate and momentum can be measured simultaneously. Let us estimate the validity domain of this approximation.

The notion of trajectory makes sense in the case of a channeling particle if one is able to determine the particle coordinate y and the transverse momentum p_y with accuracies δy and δp_y that are much smaller than the channel width d and typical value p_y^{ch} of the transverse momentum of a channeling particle. On the other hand, the product $\delta p_y \delta y$ cannot be smaller than \hbar due to the Heisenberg's uncertainty principle. We obtain, therefore, the following inequality:

$$p_y^{\text{ch}} d \gg \delta p_y \delta y > \hbar. \quad (3)$$

The transverse motion of the projectile can be described by the laws of dynamics of a nonrelativistic particle with the mass E/c^2 . Here E is the projectile energy and c is the speed of light. The transverse kinetic energy of the channeling particle cannot exceed the depth of the interplanar potential well U_{\max} :

$$\frac{(p_y^{\text{ch}})^2}{2E/c^2} < U_{\max}. \quad (4)$$

Combining (3) and (4) one sees that projectile can be considered classically if its energy E is sufficiently large:

$$E \gg \frac{(\hbar c)^2}{2d^2 U_{\max}}. \quad (5)$$

Putting $U_{\max} = 20$ eV and $d = 1$ Å one obtains $E \gg 0.1$ MeV. However, the sign \gg in this inequality has to be understood as 'at least three orders of magnitude larger'. To show this, let us consider a simple example of a parabolic potential well of depth U_{\max} and width d :

$$U(y) = U_{\max} \left(\frac{y}{d/2} \right)^2. \quad (6)$$

The oscillation frequency in such potential for a particle with the mass E/c^2 is $\omega = c\sqrt{U''(0)/E}$, where U'' is the second derivative of the potential energy with respect to y . From (6) one finds $U'' = 8U_{\max}/d$. The number of quantum levels in the potential well is

$$n \approx \frac{U_{\max}}{\hbar\omega} = \frac{d}{2\hbar c} \sqrt{\frac{U_{\max}E}{2}}. \quad (7)$$

Solving (7) for E yields

$$E \approx 16n^2 \frac{(\hbar c)^2}{2d^2 U_{\max}}. \quad (8)$$

The right hand sides of (5) and (8) coincide up to the factor of $16n^2$. The classical description is valid if the number of levels is sufficiently large. Taking $n = 10$ one obtains $16n^2 = 1600$.

Hence, our model can be always applied to ultrarelativistic heavy projectiles. It is applicable in the case of light projectiles if their energy is in hundred MeV range or higher. The applicability conditions for electron projectile may be somewhat stricter than for positrons, because the planar potential well is narrower in the case of negative particles. In the present paper we apply the model to electron projectiles at energy $E = 855$ MeV. In this case the classical approximation is expected to be satisfactory.

The process of radiation emission by the projectile is also treated classically. The energy \mathcal{E} per unit interval of radiation frequency ω per unit of solid angle Ω emitted by the projectile is calculated according to formula (14.65) from [30]:

$$\frac{d^3\mathcal{E}}{d\omega d^2\Omega} = \frac{q_p^2}{4\pi^2 c} \left| \int_{t_{\text{in}}}^{t_{\text{out}}} dt \frac{\vec{n} \times [(\vec{n} - \vec{\beta}(t)) \times \dot{\vec{\beta}}(t)]}{(1 - \vec{n} \cdot \vec{\beta}(t))^2} \exp\left\{i \frac{\omega}{c} [ct - \vec{n} \cdot \vec{r}(t)]\right\} \right|^2. \quad (9)$$

Here \vec{n} is a unit vector pointing from the crystal to a distant observation point, $\vec{r}(t)$ is the projectile coordinate as a function of time, $\vec{\beta}(t)$ and $\dot{\vec{\beta}}(t)$ are respectively its velocity and acceleration divided by the speed of light: $\vec{\beta}(t) = \dot{\vec{r}}(t)/c$, $\dot{\vec{\beta}}(t) = \ddot{\vec{r}}(t)/c$. The integration over the time t is taken from the moment t_{in} of entering to the moment t_{out} of existing the crystal by the projectile.

The classical approach is valid for relatively soft radiation: the photon energy has to be much smaller than the energy of the projectile: $\hbar\omega \ll E$.

3. Description of the Algorithm

The code performs 3D simulation of the motion of ultrarelativistic charged particles in a single crystal.

The crystal lattice is modelled as a collection of nodes. Each node is represented by the radius vector of its position and a few vectors, called ‘bonds’, connecting the node to all its nearest neighbours.

In the case of diamond-type lattice, each node has four nearest neighbours. The bond length b is calculated according to the formula

$$b = \frac{\sqrt{3}}{2}v^{1/3}, \quad (10)$$

where v of the volume per atom:

$$v = \frac{A}{\rho N_A}. \quad (11)$$

Here A is the atomic weight, ρ is the density of the crystal and N_A is the Avogadro constant.

The lattice is built as follows. A node is placed at the origin of the coordinate system. The ‘bonds’ of this node are oriented as described below. Then the lattice is ‘grown’ by placing new nodes at free ends of the ‘bonds’ until the necessary space region is filled with the lattice.

To study the channeling along the crystallographic plane defined by the Miller indices (klm) the lattice has to be oriented in such a way that its (klm) plane is parallel to the coordinate plane (xz) , where z is the beam direction. This is accomplished by the proper orientation of the ‘bonds’ of the initial node. At the beginning, the ‘bonds’ of the initial node are

$$\vec{b}_1 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}) \quad (12)$$

$$\vec{b}_2 = (1/\sqrt{3}, -1/\sqrt{3}, -1/\sqrt{3}) \quad (13)$$

$$\vec{b}_3 = (-1/\sqrt{3}, 1/\sqrt{3}, -1/\sqrt{3}) \quad (14)$$

$$\vec{b}_4 = (-1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3}). \quad (15)$$

It corresponds to the orientation of the crystallographic directions $[100]$, $[010]$ and $[001]$ along the axes x , y and z , respectively. Then a rotation matrix $O_{(klm)}$ is built that

transforms the vector (k,l,m) into the vector of the same length directed along the y -axis. All four ‘bonds’ (12)–(15) are multiplied by this matrix: $\vec{b}_i \rightarrow O_{(klm)}\vec{b}_i$, $i = 1, 2, 3, 4$. Finally the ‘bonds’ are also multiplied by the rotation matrix O_ϕ describing rotation around the y -axis by the angle ϕ . The angle ϕ has to be carefully chosen to avoid collinearity of major crystal axes with the coordinate axis z .

In a similar way, a crystal axis can be oriented along the beam direction z to simulate axial channeling.

There is also a possibility of a random orientation of the crystal avoiding incidental orientation of major crystal directions along the beam axis. In this case the crystal scatters particles as an amorphous medium. This regime can be used to calculate the incoherent bremsstrahlung.

Once the lattice is constructed, the atoms are placed in its nodes. Each atom is a collection of electric charges: a nucleus with the charge $+Ze$ and Z electrons with charges $-e$, $Z = 14$ in the case of silicon. The positions of the electrons are random. Their distribution is spherically symmetric and the distance of electrons from the nucleus is calculated as

$$r_i = a_{\text{TF}}\hat{r}_i, \quad i = 1, \dots, Z. \quad (16)$$

Here, a_{TF} is the Thomas-Fermi radius of the atom:

$$a_{\text{TF}} = \frac{0.8853}{Z^{1/3}}a_{\text{B}}, \quad (17)$$

with a_{B} being Bohr’s radius, and \hat{r}_i is found by solving the following transcendental equation

$$\chi(\hat{r}_i) - \hat{r}_i\chi'(\hat{r}_i) = \xi_i \quad (18)$$

with ξ_i being a random variable uniformly distributed within the interval $0 < \xi_i \leq 1$. The function $\chi(\hat{r})$ in (18) is the screening function of the atomic potential. It can be shown that, if the positions of electrons are chosen as described above, the total electrostatic potential of the nucleus and the electrons being averaged over the random positions of the electrons has the form

$$\langle U(r) \rangle = \frac{Ze}{r} \chi\left(\frac{r}{a_{\text{TF}}}\right). \quad (19)$$

The screening function $\chi(\hat{r})$ satisfies the conditions

$$\xi(0) = 1, \quad \lim_{\hat{r} \rightarrow +\infty} \chi(\hat{r}) = 0, \quad (20)$$

so that the potential has the Coulomb form $(Ze)/r$ in the vicinity of the nucleus but is fully screened out by the electron cloud at large r .

We use the Molière screening function [28], which has the form

$$\chi(\hat{r}) = \sum_{j=1}^3 \alpha_j \exp(-\beta_j \hat{r}) \quad (21)$$

with numerical parameters having the values

$$\begin{aligned} \alpha_1 &= 0.35, & \alpha_2 &= 0.55, & \alpha_3 &= 0.1, \\ \beta_1 &= 0.3, & \beta_2 &= 1.2, & \beta_3 &= 6.0. \end{aligned} \quad (22)$$

To take into account quantum and thermal oscillations of the atoms in the crystal, the atomic nucleus is placed not exactly in the lattice node but is shifted from it by a random vector $\vec{\rho}$. Each component of the random vector is normally distributed:

$$w(\rho_k) = \frac{1}{\sqrt{2\pi}a(T)} \exp \left[-\frac{1}{2} \left(\frac{\rho_k}{a(T)} \right)^2 \right], \quad k = x, y, z \quad (23)$$

Here $a(T)$ is the average oscillation amplitude. We used the value $a(T) = 0.075 \text{ \AA}$ in our calculations, which corresponds to the room temperature [31].

The trajectory of the projectile is modelled as follows: The particle moves along straight line segments between the points where its coordinate z coincides with the z coordinate of one of a crystal constituent: an electron or a nucleus. At this point the transverse momentum of the projectile is changed according to equation (2). Then the projectile is moved further along a straight line segment corresponding to the transverse momentum $\vec{p}_\perp + \Delta\vec{p}_\perp$ until its z coordinates coincides with that of the next crystal constituent and a new modification of the particle momentum is performed.

A crystal constituent is taken into account if it belongs to the lattice node located within a cylinder of the radius $40a_{\text{TF}}$ around the particle. Initially, the axis of the cylinder is the straight line along the direction of the projectile momentum at the point of entering the crystal. The length of the cylinder is approximately 200 \AA . When the particle approaches the end of the cylinder, a new cylinder is built as an extension of the old one but along the direction of the new particle momentum. The procedure continues until the end of the crystal is reached. As result, the cylinders form a ‘pipe’ filled by the crystal lattice and the particle channels inside it as it is shown in Figure 2. The computer time is saved substantially due to the fact that only the part of the crystal lattice inside the ‘pipe’ is modelled and the rest of it is ignored.

After the projectile trajectory is simulated, the radiation spectrum is calculated. The integral in (24) is approximated with a sum over the trajectory points:

$$\frac{d^3\mathcal{E}}{d(\hbar\omega)d^2\Omega} = \frac{\alpha}{4\pi^2} \left| \sum_j \left(\frac{\delta\vec{\beta}_j}{D_{j-1}} + \frac{(\vec{\beta}_j - \vec{n})(\delta\vec{\beta}_j \cdot \vec{n})}{D_j D_{j-1}} \right) \exp \left(i \frac{\phi_{j-1} + \phi_j}{2} \right) \right|^2, \quad (24)$$

where $\delta\vec{\beta}_j$ is an increment of $\vec{\beta}$ between two successive trajectory points: $\delta\vec{\beta}_j = \vec{\beta}_j - \vec{\beta}_{j-1}$ and α is the fine structure constant. The denominators D_j are found from the formula $D_j = 1 - (\vec{\beta}_j \cdot \vec{n})$ and the phases ϕ_j are given by the expression

$$\phi_j = \frac{\omega}{c} [ct_j - \vec{n} \cdot \vec{r}_j]. \quad (25)$$

Dividing (24) by $\hbar\omega$ yields the formula for the number of photons.

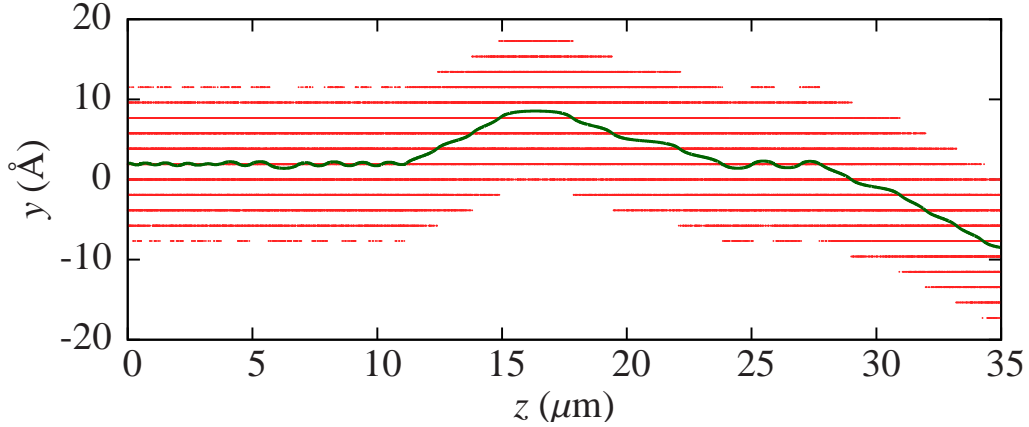


Figure 2. An example of the crystal ‘pipe’ surrounding the particle trajectory as it is modelled by the code. A projection on plane (zy) is shown.

4. Simulations

The calculations were performed for $E=855$ MeV electrons in a single crystal of silicon for three crystal orientations corresponding to channeling along (100), (110) and (111) planes. The simulated positions of the crystal constituents and the potential energy of the projectile electron in the electrostatic field of crystal planes are shown in Figure 3.

Initially, the projectiles had zero transverse momentum. This corresponds to the ideal case of a zero-emittance beam entering the crystal strictly parallel to the coordinate axis z . The transverse position of the projectile at the entrance of the crystal was chosen randomly, homogeneously distributed along the channel width. Then the trajectory of the particle was simulated as it is described in the previous section. The simulation of the trajectory was terminated if the particle went through the crystal: $z > L_{\text{cr}}$, or if the deviation of the projectile from its initial direction became too large: $|\vec{p}_{\perp}|/p_z > 100/\gamma$ (here p_{\perp} and p are respectively the transverse and the longitudinal momenta and γ is the Lorentz factor of the projectile.)

Each simulated trajectory was analysed to determine the segments of the trajectory corresponding to the channeling and dechanneling regime. The particle was considered to be in the channeling regime if it changed the direction of the y component of its velocity two or more times without crossing the channel boundaries, i.e. if it made at least one complete channeling oscillation. After crossing the boundary of the channel, the particle was considered to be dechanneled until it performed another full channeling oscillation or until terminating the simulation of the trajectory.

The number of the simulated trajectories for the analysis of dechanneling was 40000, 30000 and about 28000 for planar channels (111), (110) and (100), respectively. The dimension of the crystal in the beam direction L_{cr} was equal to maximum length of the crystals used in recent channeling experiments [27]: $L_{\text{cr}} = 270.4 \mu\text{m}$.

Channeling radiation was calculated for the plane (110) and for ‘amorphous’ orientation (i.e. for a crystal oriented randomly avoiding major crystal directions) for

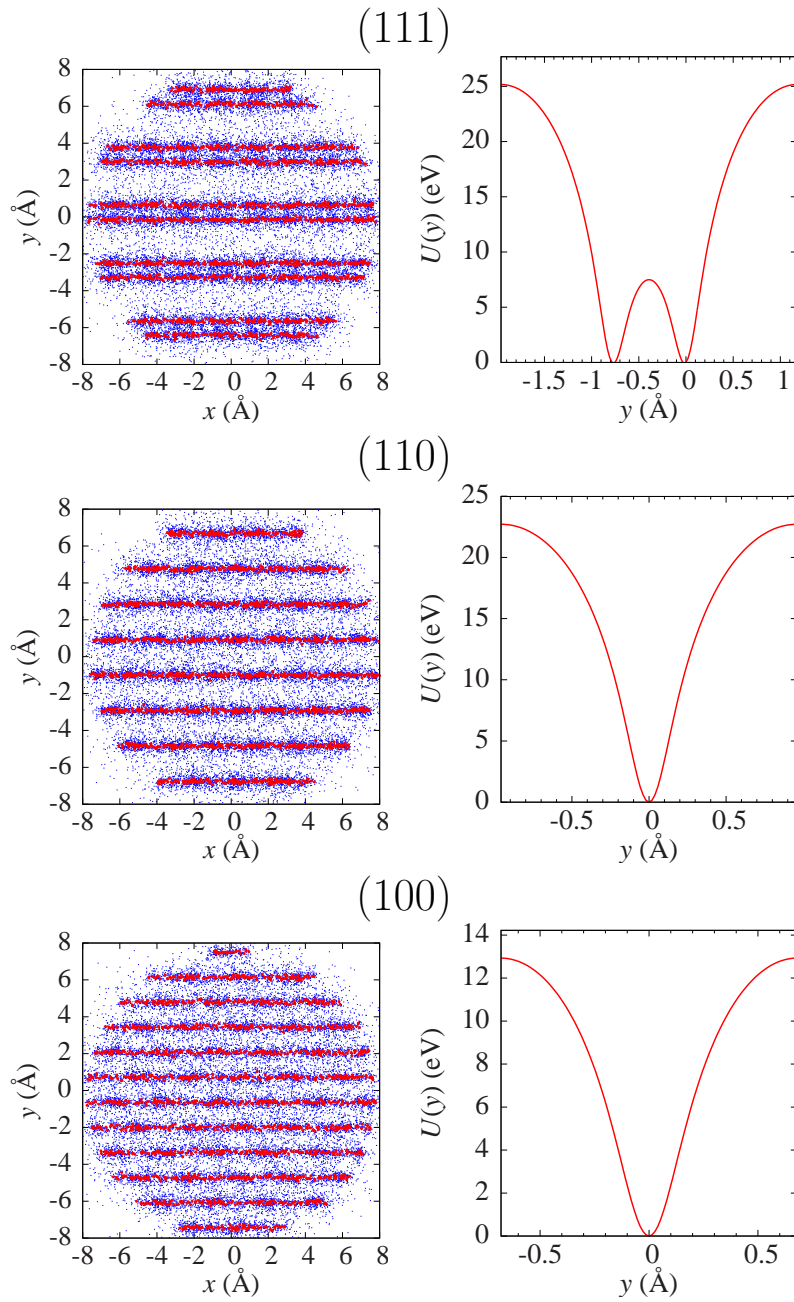


Figure 3. Left column: The projection of a 200 Å long simulated crystal cylinder on the (xy) plane. Smaller and larger circles stand respectively for electrons and nuclei. Right column: the potential energy of the projectile electron in the field of crystal planes in continuous approximation. The plots in right column serve an illustrative purpose only, the continuous potentials are not used in the calculation algorithm.

seven different values of L_{cr} ranging from $L_{\text{cr}} = 7.9 \mu\text{m}$ to $L_{\text{cr}} = 270.4 \mu\text{m}$, 50000 trajectories were simulated in each case.

5. Definition of the Dechanneling Length

To make a quantitative assessment of the particle dechanneling process, one needs a definition of the dechanneling length that would be suitable for the Monte Carlo approach.

Let z_{d1} be the point of the first dechanneling of the projectile. We define the quantity $N_{\text{ch0}}(z)$ as the number of projectile particles for which $z_{\text{d1}} > z$, i.e. this is the number of particles that passed the distance from the crystal entrance to the point z in the channeling regime and dechannel at some further point. The length $L(z)$ is the average distance from the point z to the first dechanneling point:

$$L(z) = \frac{\sum_{k=1}^{N_{\text{ch0}}(z)} (z_{\text{d1}}^{(k)} - z)}{N_{\text{ch0}}(z)}. \quad (26)$$

The sum in the numerator of is taken over those projectiles for which $z_{\text{d1}} > z$.

Generally speaking, $L(z)$ depends not only on z , but also on the angular distribution of the particles at the crystal entrance. Nonetheless, as it will be shown below, the kinetic theory of channeling suggests that, at sufficiently large z , $L(z)$ reaches an asymptotic value that depends neither on z nor on the initial angular distribution.

From the solution of the diffusion equation (see, for instance, formula (1.38) in [32]), one can obtain the following expression for $N_{\text{ch0}}(z)$

$$N_{\text{ch0}}(z) = N_0 \sum_{j=1}^{\infty} a_j \exp(-z/L_j). \quad (27)$$

Here only coefficients a_j depend on the initial angular distribution of the particles, while the lengths L_j depend exclusively on the properties of the crystal channel and the energy, charge and mass of the projectile.

The dechanneling length L_d is defined as the largest of the parameters L_j in (27). The corresponding term dominates the asymptotic behaviour at $z \gtrsim L_d$:

$$N_{\text{ch0}}(z) \asymp N_0 a_d \exp(-z/L_d). \quad (28)$$

The expression (26) for $L(z)$ has the following counterpart in the kinetic theory

$$L(z) = \frac{1}{N_{\text{ch0}}(z)} \int_z^{\infty} dz_{\text{d1}} (z_{\text{d1}} - z) N_{\text{ch0}}(z_{\text{d1}}) \quad (29)$$

Substituting (28) into (29) demonstrates that, indeed, the coefficient a_d cancels out and $L(z)$ becomes equal to L_d in the asymptotic region.

Although the diffusion equation was solved in [32] for positively charged projectile in harmonic potential approximation, the exponential asymptotic behaviour of $N_{\text{ch0}}(z)$, and, consequently, a constant asymptotic value of $L(z)$ is a more general result. As it will be shown in the next section, our simulations demonstrate that it is also valid for electrons.

Hence, in our Monte Carlo procedure the dechanneling length L_d is defined as the asymptotic value of $L(z)$ in the region where it ceases to depend on z .

6. Analysis of the Results

The ratio $N_{\text{ch0}}(z)/N_0$ as function of z is shown in Figure 4 for three different crystal channels. This fraction decreases rather fast and, as it was expected, has an exponential

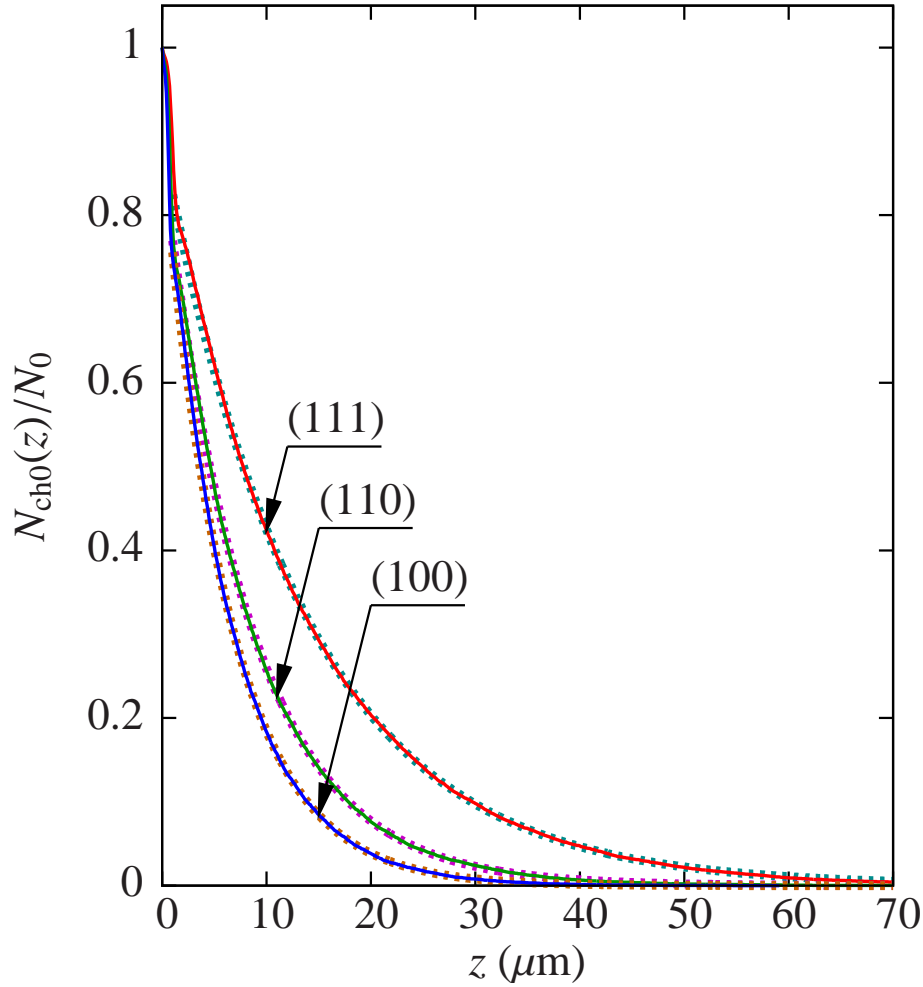


Figure 4. Fraction $N_{\text{ch0}}(z)/N_0$ of the particles that stay in the same channel from their entrance into the crystal for different planar channels as function of the penetration depth z . The thick dashed lines show the corresponding exponential asymptotes $\propto \exp(-z/L_d)$, the values of L_d are listed in Table 1.

asymptotic behaviour.

The quantity $L(z)$ (26) for the same channels is plotted in Figure 5. Indeed, $L(z)$ becomes constant (within the statistical errors) at large z corresponding to exponential behaviour of the curves of Figure 4. The asymptotic values, L_d , are listed in Table 1.

Only the particles that remained in the channeling regime from their entrance to the crystal were considered in Figures 4 and 5. The fraction of these particles decreases

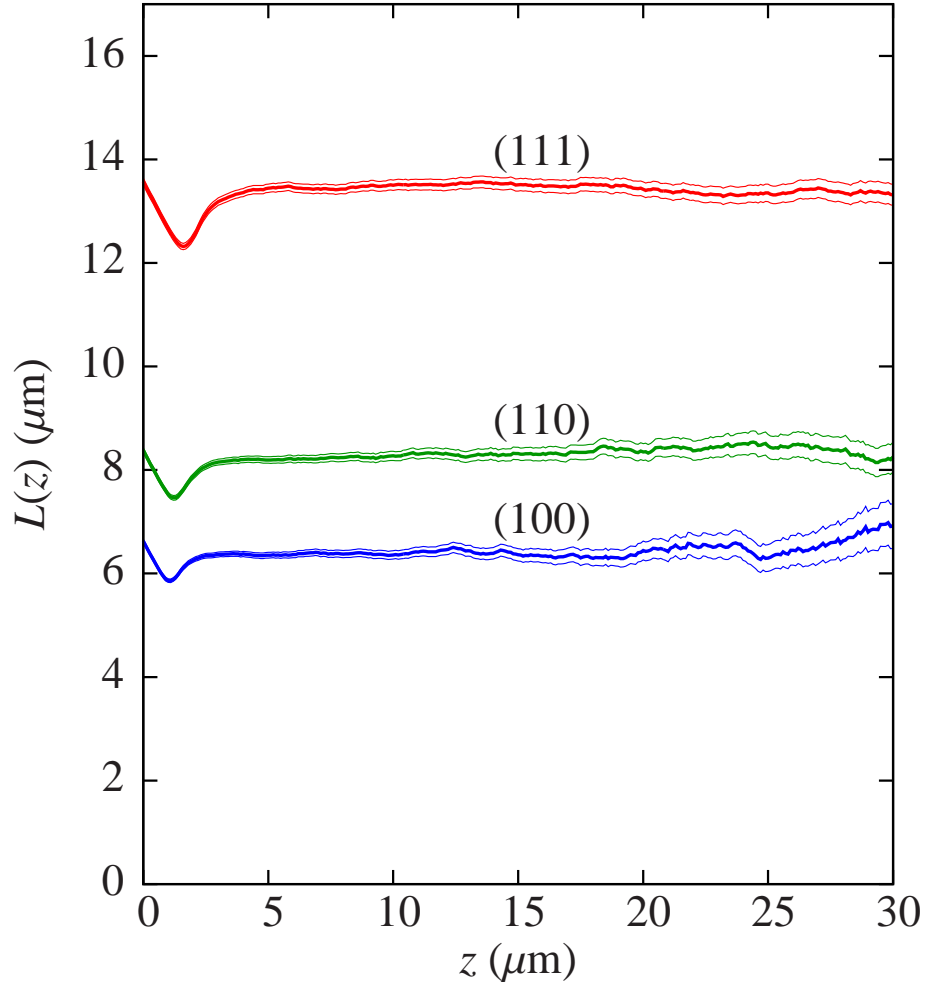


Figure 5. The quantity $L(z)$ (26) that becomes equal to the dechanneling length at large penetration depth z . The thin lines show the statistical errors.

Table 1. Monte Carlo results for the dechanneling length L_d for three different crystal channels. The results for initial beam and rechanneled particles coincide within the statistical errors.

Crystal Plane	Dechanneling Length (μm)	
	Initial beam	Rechanneled particles
(111)	13.57 ± 0.12	13.69 ± 0.07
(110)	8.26 ± 0.08	8.38 ± 0.05
(100)	6.38 ± 0.07	6.40 ± 0.05

fast. In contrast, the fraction $N_{\text{ich}}(z)/N_0$ of the particles that are in the channeling regime at the point z regardless of their previous channeling status decreases rather slowly (see Figure 6). The reason for it is the rechanneling process. Random collisions with the crystal constituents can occasionally reduce the transverse energy

$$E_y = \frac{p_y^2}{2E/c^2} + U(y). \quad (30)$$

Therefore, a dechanneled particle can return to the channeling regime.

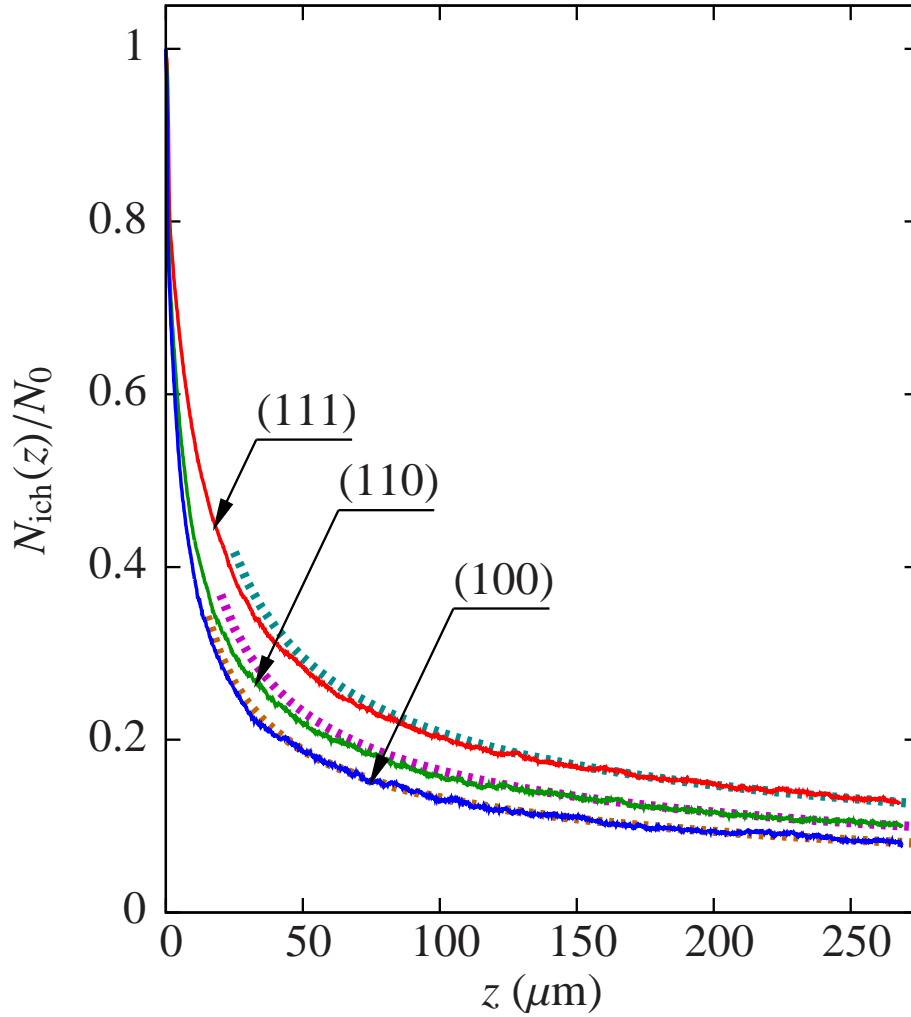


Figure 6. The fraction of channeling particles as function of penetration depth z for different crystal channels (solid lines). The thick dashed lines show the corresponding asymptotes $\propto z^{-1/2}$.

Rechanneling occurs more often for electrons than for positively charged particles. This is due to the fact that the random scattering is more intense in the vicinity of the crystal plane. For positively charged particles this means that the scattering is most probable at the top of the potential barrier, i.e. near the maximum of the potential energy $U(y)$. Even if a collision happens to reduce the component p_y of the projectile

momentum to zero, the transverse energy E_y still remains in the vicinity of the top of the potential barrier. The range of p_y at which the particle returns to the channeling regime is zero at the maximum of the potential and is small in the vicinity of it. Therefore, probability of the rechanneling is small.

In contrast, the potential minimum for negatively charged particles is located near the crystal planes. This means that the random collisions are most probable near the minimum of the potential energy, where there is a wider range of p_y at which E_y drops below the potential barrier. Hence, the probability of rechanneling is higher for negative than for positive particles.

Typical trajectories of electrons are shown in Figure 7, where rechanneling is clearly

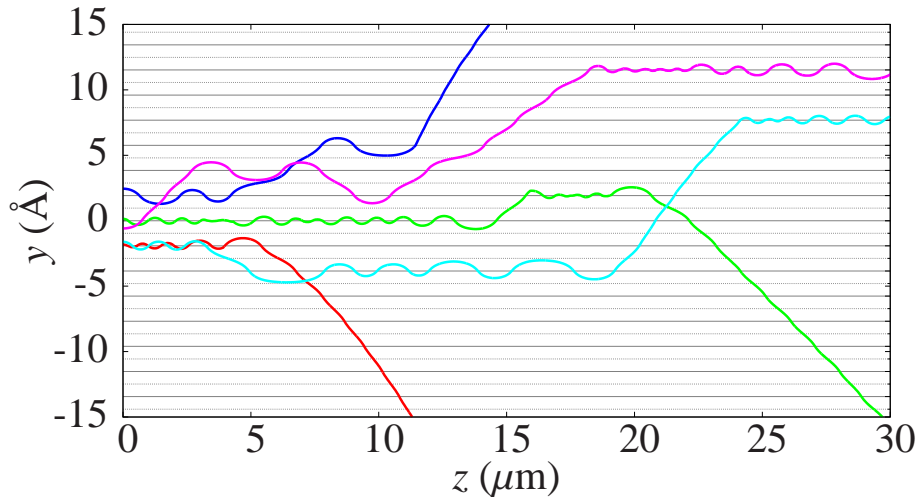


Figure 7. Examples of simulated trajectories. Only initial segments corresponding to $z < 30 \mu\text{m}$ are plotted. The crystallographic planes are shown by solid horizontal lines, dashed lines show the boundaries between the channels (the maxima of the interplanar potential). Four of five trajectories demonstrate rechanneling. One of the particles rechannels twice.

seen. According to our results, a particle rechannels in average 4.8 times on the length of the crystal $L_{\text{cr}} = 270.4 \mu\text{m}$ into the channel (100). For the channels (110) and (111) the corresponding numbers are respectively 4.4 and 3.5.

The asymptotic behaviour of the curves in Figure 6 can be explained in the following way. At sufficiently large z , the distribution of the dechanneled particles with respect to the transverse momentum p_y is similar to that in an amorphous medium and can be approximated by the Gaussian function:

$$w(p_y) = \frac{1}{\sqrt{2\pi}\sigma(z)} \exp \left[-\frac{1}{2} \left(\frac{p_y}{\sigma(z)} \right)^2 \right] \quad (31)$$

with the variance proportional to z : $\sigma^2(z) \propto z$. The rechanneling is dominated by the phase space density the vicinity of the point $p_y = 0$. It decreases as $1/\sigma(z) \propto 1/\sqrt{z}$ and governs the asymptotic behaviour of the fraction of the channeling particles shown in Fig. 6.

For the analysis of the rechanneled particles, one can consider the quantity $N_{\text{chn}}(\tilde{z})$, which is the number of particle that rechanneled at least n times and travelled at least the distance \tilde{z} from the n -th rechanneling point z_{rn} in the channeling regime, i.e. this is the number of particles for which

$$z_{\text{d}(n+1)} - z_{\text{rn}} > \tilde{z}, \quad (32)$$

where $z_{\text{d}(n+1)}$ is the point of $(n+1)$ -th dechanneling. Note that the longer is the crystal along the beam direction the larger is the probability of rechanneling, therefore $N_{\text{chn}}(\tilde{z})$ for $n > 0$ depend on L_{cr} , in contrast to N_{ch0} .

It is reasonable to expect that the particle ‘forgets’ the value of its initial transverse momentum by the point of its first rechanneling or even earlier. Therefore, all the rechannelings (1st, 2nd, and so on) are expected to be statistically identical and it makes sense to analyse them together. We introduce the quantity

$$N_{\text{rch}}(\tilde{z}) = N_{\text{ch1}}(\tilde{z}) + N_{\text{ch2}}(\tilde{z}) + N_{\text{ch3}}(\tilde{z}) + \dots \quad (33)$$

Note that $N_{\text{rch}}(\tilde{z})$ may be larger than the total number of particles N_0 , because each particle may rechannel several times.

The ratio $N_{\text{rch}}(\tilde{z})/N_0$ for $L_{\text{cr}} = 270.4 \mu\text{m}$ for three crystal channels is plotted in Figure 8. Similarly to $N_{\text{ch0}}(z)$, this quantity decreases fast with \tilde{z} and has an exponential asymptote.

It is possible to introduce the quantity $L(\tilde{z})$, which is a counterpart of (26) for rechanneled particles:

$$L(\tilde{z}) = \frac{\sum_k \sum_n (z_{\text{d}(n+1)}^{(k)} - z_{\text{rn}}^{(k)} - \tilde{z})}{N_{\text{rch}}(\tilde{z})}. \quad (34)$$

The first sum in the numerator runs over all particles that rechanneled at least once. The second sum runs over all rechannelings of each particle.

The quantity $L(\tilde{z})$ is plotted in Figure 9. The behaviour of $L(\tilde{z})$ and $L(z)$ (see Figure 5) at small values of \tilde{z} and z is different, because the transverse momentum distribution of the rechanneling particles is quite different from that of the ideally parallel initial beam. But asymptotic behaviour of both quantities is essentially the same: they both reach a constant value, which is, by definition, the dechanneling length L_{d} . In Table 1, the values of L_{d} obtained from the analysis of rechanneled particles is compared to those obtained for the initial beam. They coincide within the statistical errors. This confirms that the dechanneling length calculated according to our definition does not depend on the initial transverse momentum distribution of the projectiles.

7. Comparison to Experiment

The dechanneling length cannot be measured directly in an experiment because it is not possible to separate the particles that were in the channeling regime from the entrance point and the rechanneled particles. Only signals related to the total number of channeling particles can be measured. Extracting the dechanneling length

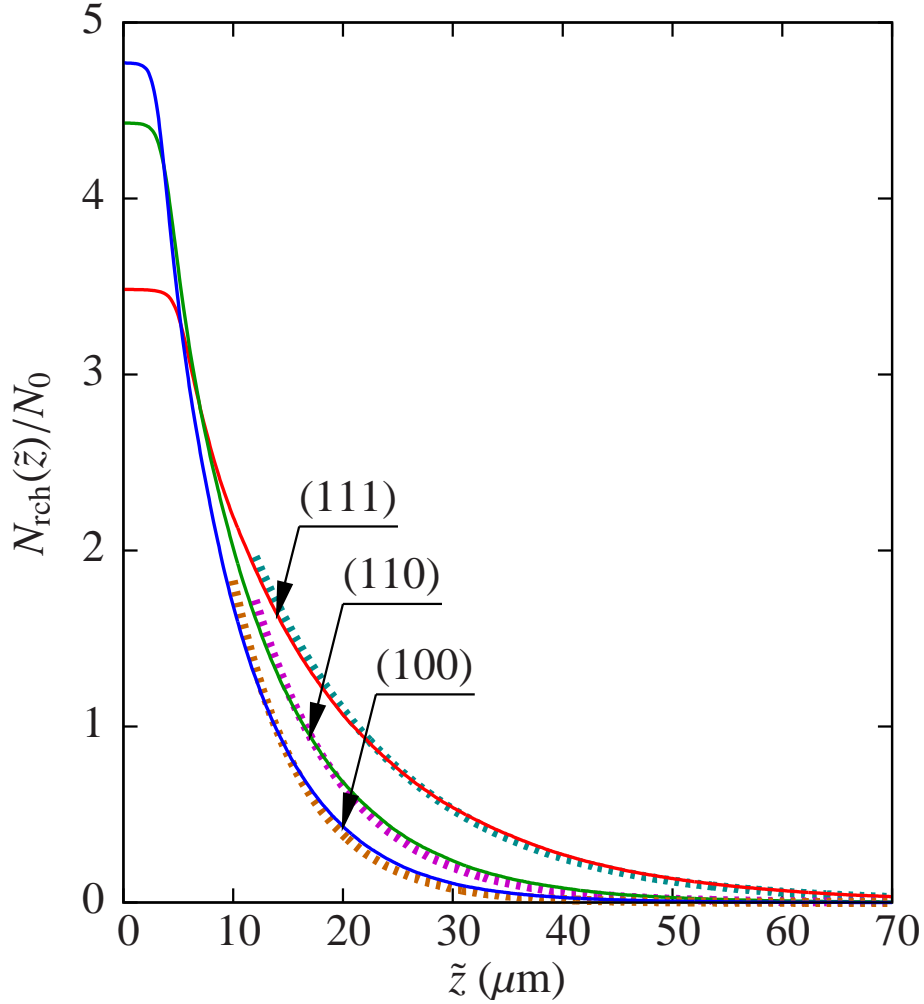


Figure 8. The ratio $N_{\text{rch}}(\tilde{z})/N_0$ (see text) for different planar channels as function of the distance \tilde{z} from the rechanneling point. The thick dashed lines show the corresponding exponential asymptotes $\propto \exp(-z/L_d)$, the values of L_d are listed in Table 1.

from these data involves a model-dependent procedure. Therefore, comparing the values of L_d obtained by Monte Carlo simulations to estimations found in the experimental publications would be a comparison of two theoretical models rather than an experimental verification of the code.

A correct way to check a physical model and the corresponding computer code is to use it for calculation of those quantities that can be directly measured in an experiment. Then these results should be compared to the experimental data.

In the experiment at Mainz Microtron [27] the intensity of the channeling radiation was measured for crystal samples of different dimensions L_{cr} along the beam axis. To make a comparison with these data, we modelled the Mainz experiment with our code.

We calculated the average number of photons in the energy interval $0.4 \text{ MeV} < \hbar\omega < 9.0 \text{ MeV}$ emitted by a 855 MeV electron moving through a Silicon crystal with

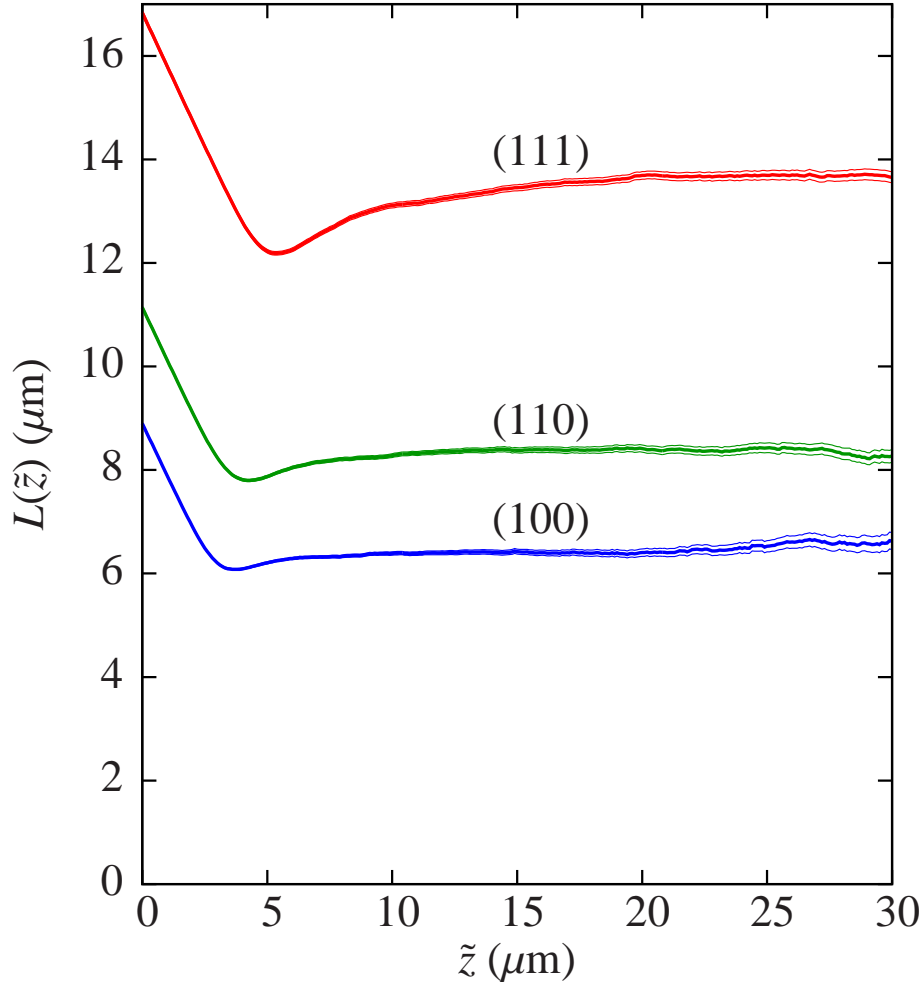


Figure 9. The quantity $L(\tilde{z})$ (34) for different planar channels as function of the distance \tilde{z} from the rechanneling point. The thin lines show the statistical errors. Note that the asymptotic values of $L(\tilde{z})$ are the same as for $L(z)$ (cf. Figure 5).

plane (110) parallel to the beam direction. Then we subtracted the background, i.e. the same quantity but calculated in the case of a randomly oriented Silicon crystal. The photons were taken into account if the angle θ between their wave vector and the beam direction, does not exceed 1.31 mrad, which corresponds to the aperture of the gamma spectrometer in the experimental setup of the Mainz experiment. The calculation were done for different values of L_{cr} .

The intensity of the channeling radiation is presented in [27] in arbitrary units. We equated 12 arbitrary unit to 1 photon per projectile to adjust the overall scale. The results are shown in Figure 10. As is seen, our results demonstrate reasonable agreement with the experiment, which proves the reliability of the code.

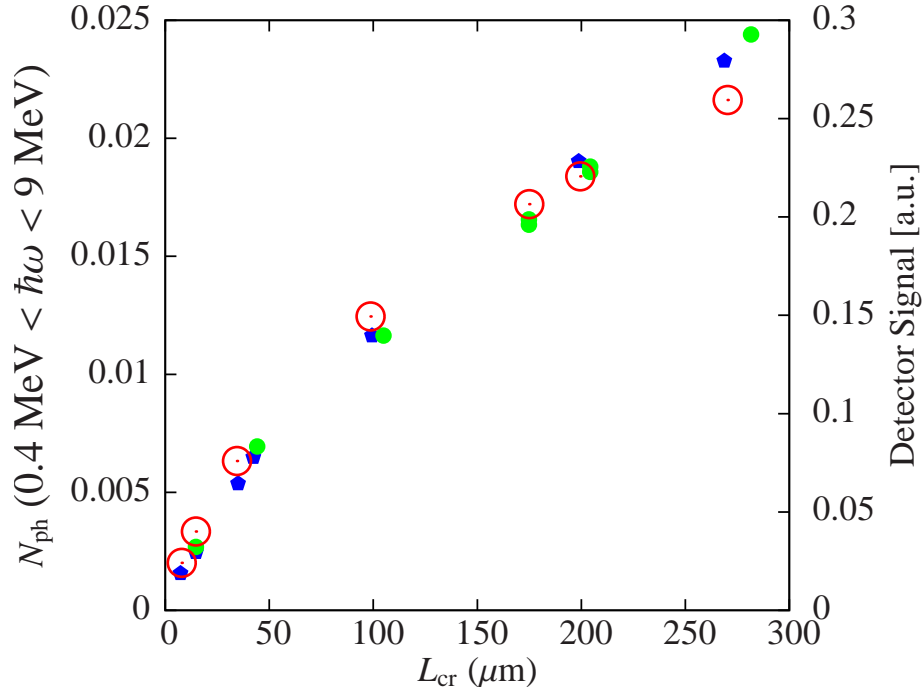


Figure 10. Channeling radiation as function of crystal size along the beam direction. The filled symbols are experimental data [27] and the open cycles are results of our calculations. The left vertical axis shows the number of emitted photons per projectile within the energy interval $0.4 \text{ MeV} < \hbar\omega < 9.0 \text{ MeV}$. The right vertical axis is calibrated in arbitrary units used in the experimental paper.

8. Conclusion and Discussion

We presented first result obtained with a new Monte-Carlo code for modelling of channeling of ultrarelativistic charged particles in a crystal. The calculation were done for 855 MeV electrons channeling in a single crystal of Silicon along (100), (110) and (111) crystallographic planes.

According to our simulation, if rechanneling is disregarded, the number of channeling electrons decreases fast with the penetration depth z and quickly approaches an exponential asymptote. Similar behaviour was previously seen in the kinetic theory of channeling in the case of positively charged projectile.

We formulated a definition of the dechanneling length L_d that is suitable for application within the Monte Carlo approach. Our definition is consistent with the one previously used in the kinetic theory of channeling. Applying this definition to the initial beam and to rechanneled particles gives essentially the same result. This demonstrates that L_d is a universal quantity and does not depend on the initial transverse momentum distribution of projectiles.

We calculated the dechanneling length for the studied planar channels. It appeared to be in the $10 \mu m$ range.

Our simulations show that the rechanneling of electrons is a notable phenomenon.

It dominates the number of channeling particles already at the penetration depth of a few tens of microns. Due to rechanneling, the total number of channeling particles, included the rechanneled fraction, decreases slowly following the $\propto 1/\sqrt{z}$ asymptote.

To verify our code, we calculated the intensity of the channeling radiation and compared it with the experimental data obtained at Mainz Microtron [27]. A good agreement has been observed. This confirms that our code is a reliable tool for modeling the electron channeling if the projectile energy is around 1 GeV.

There is no obstacle for successful application of the code also to positrons of the same energy range or to electrons and positrons of higher energy up to several tens of GeV. Extending the applicability domain of the code to much lower or to much higher projectile energies requires further improvements of the underlying physical model and the computation algorithm.

At low projectile energies (around 100 MeV or lower) the splitting of the transverse energy levels of a channeling electron or positron can be as large as a few electronvolts, which is comparable with the depth of the potential well. Because only discrete transverse energy levels are allowed, scattering from the crystal constituents will lead to an increase of the transverse energy only when the energy transfer in the collision is equal to the splitting. Hence, only collisions with large scattering angles can contribute to the increase of transverse energy. Due to smaller probability of such collisions, the dechanneling length may become noticeably larger than it is predicted by classical calculations. For these reasons, a study of low energy electron and positron channeling would require taking into account quantum properties of the projectile.

At high electron or positron energies (hundreds of GeV or higher), the radiation energy losses become essential and cannot be ignored. Therefore, our model has to be further developed to take these into account.

In the case of heavy projectiles, the radiation energy losses are much less important. Therefore, in principle, our model can be applied to heavy projectiles of TeV energy range or even higher. However, calculations of heavy projectile channeling may involve very long crystals because of a large dechanneling length. This could require a prohibitive amount of computer time. Therefore, further refinement and optimisation of the algorithm may be necessary in this case.

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